Theoretical Investigation of Spectroscopic, Electronic and Thermodynamic Properties of [2-Methoxy-4-(3-methyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl)-azomethinphenyl] Acetate Molecule

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Authors' contributions

This work was carried out in collaboration between all authors. Author HY designed the study, managed the literature searches and interpreted all spectroscopic and experimental results. Author GK wrote the protocol and performed all theoretical studies. Author GO wrote the first draft of the manuscript and interpreted the theoretical results of the study. All authors read and approved the final manuscript.

Original Research Article

ABSTRACT

Firstly, [2-Methoxy-4-(3-methyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl)-azomethinphenyl] acetate molecule was optimized by using Density Functional Theory (DFT/B3LYP) and Hatree Fock (HF/B3LYP) methods. Then, from this the most stable structure of the optimized molecule the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), bond lengths, bond angles, mulliken charges, E_{LUMO}-E_{HOMO} energy gap (ΔEg), electronegativity (χ), electron affinity (A), global hardness (η), softness (σ), ionization potential (I), total energy of the molecule, dipole moments and thermodynamic properties were calculated with B3LYP/631G (d) and HF/631G (d) basis sets. Otherwise, the veda4f program was used in defining IR data, which were theoretically calculated. Experimental data obtained from the literature. The experimental and the calculated theoretical values were compared. Theoretically calculated IR data are multiplied with

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appropriate adjustment factors and the data obtained according to DFT and HF method are formed using theoretical infrared spectrum. Finally, ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated with the method of GIAO using the program package Gaussian G09. Experimental and theoretical values of the investigated molecule were inserted into the graphic according to equation of δ exp‗a+b. δ calc. The standard error values were found via SigmaPlot program with a regression coefficient of a and b constants.

1. INTRODUCTION

Schiff bases are synthesized by condensation between a primary amine and an aldehyde or ketone to form an imine or azomethine (-CH=N-) group [1]. A Schiff base is a nitrogen analogue of an aldehyde or ketone in which the C=O group is modified by C=N-R group. These compounds are usually formed by reaction of an aldehyde with a primary amine, where R, may be an alkyl or an aryl group. Schiff bases that include aryl substituents are fundamentally more stable and more easily synthesized, while those which contain alkyl substituents are comparatively unstable. 1,2,4-triazole and its derivatives are an important class of organic compounds with diverse medicinal applications such as anticonvulsant, antiinflammatory, anticancer, antibacterial, anti-HIV, anti-viral, antitumor, antiphlogistic, antiallergic, antibiotics, antifungal, antioxidant properties [2-5] and as intermediates for many bioactive molecules [6,7]. The improve of computational chemistry has been used in the providence of many properties in the chemical systems. Rather, theoretical calculations provide a contribution to spectroscopic studies that are carried out largely experimentally [8-13]. Many studies have lately been made using Schiff bases [14–18]. Recently, the theoretical studies of Shiff bases have been carried out. In this study, we investigated theoretical features of [2-Methoxy-4-(3-methyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one-4-yl)-azomethinphenyl] acetate molecule. All theoretical calculations for the target compound were with the Gaussian 09 quantum chemistry program [19] on a personal computer. For this, firstly, the molecule was optimized by using the Density Functional Theory (DFT) and Hatree Fock (HF) methods with the restricted B3LYP [19,20] level of theory, 6-31G(d) basis set, for all atoms. Optimized structure is the most stable structure of the molecule. Then from this form, dipole moments, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), total energy of the molecule, bond lengths and mulliken charges, electronic properties; E_{LUMO}-E_{HOMO} energy gap (ΔEg),

electronegativity (χ), electron affinity (A), global hardness (η), softness (σ), ionization potential (I), thermodynamics properties; (thermal energies (E), thermal capacity (CV), entropy (S) were calculated. In addition, The theoretical calculations ^{1}H-NMR and ^{13}C-NMR were performed by using DFT and HF with the B3LYP/6-31G(d) level. ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09 [20]. Theoretical and experimental values [21] were inserted into the graphic according to equation of δ exp‗a+b. δ calc. The standard error values were found via SigmaPlot program with a regression coefficient of a and b constants. Finally, the theoretical vibrational spectra were calculated at the B3LYP/DFT/HF 6-31G(d) basis set in the gas phase and these data are scaled with 0.9613 and 0,8929 factors [22]. The data obtained according to DFT and HF method are formed using theoretical infrared spectrum. The theoretical IR spectra are given in Fig. 3. The veda4f program was used in defining IR data [23].

2. MATERIALS AND METHODS

2.1 Experimental

Experimental data of the molecule was obtained from the literature [21]. Melting points were check on WRS-2A Microprocessor Melting-Point Apparatus. The IR spectra were measured on Alpha-P Bruker FT-IR Spectrometer. ^{1}H- and ^{13}C-NMR spectra were recorded in deuterated dimethyl sulfoxide with TMS as internal standard on a Bruker 400 MHz spectrometer, respectively. UV absorption spectra were measured in 10-mm quartz cells between 200 and 400 nm using a PG Instruments Ltd T80 UV-vis Spectrometer. Extinction coefficients (ε) are expressed in L·mol^{-1}·cm^{-1}. Yield: 97%, m.p. 195-6°C. IR (u, cm-1): 3183 (NH), 1770, 1700 (C=O), 1596, 1578 (C=N), 1267 (COO). ^{1}H- NMR (DMSO-d6): δ 2.24 (s, 3H, CH3), 2.30 (s, 3H, OCOCH3), 3.80 (s, 3H, OCH3), 6.83-7.51 (m, 3H, ArH), 9.80 (s, 1H, N=CH), 11.78 (s,1H, NH). ^{13}C-NMR (DMSO-d*6*): δ 11.77 (CH3), 20.77 (OCOCH3), 56.27

(OCH3), 118.13, 119.89, 127.58, 127.68, 144.87, 152.10 (from-C), 144.90 (triazole C3), 148.93 (N=CH), 151.99 (triazole C5), 169.05 (COO).

2.2 Theoretical

The quantum chemical calculations were carried out with density functional theory (DFT) and Hartree-Fock (HF) methods using 6-31G (d) basis set at the Gaussian 09W program package on a computing system [19]. Firstly, the compound was optimized by using the B3LYP/6-31G (d) and HF/6-31G (d) basis sets [19,20]. Thus, the most stable geometrical conformer of the compound was obtained. Then, ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated with the method of GIAO [20]. The veda4f program was used in defining IR data [23]. Theoretically calculated IR data are multiplied by appropriate adjustment factors [22]. Scale dft and hf values obtained according to HF and DFT method are formed using theoretical infrared spectrum. Otherwise, bond angles, bond lengths, the HOMO-LUMO energy and mulliken charges of the compound were calculated theoretically on the computer. The temperature addicted thermodynamic parameters (thermal energies **E**, thermal capacity **CV**, entropy **S**) were calculated from the vibrational frequency calculations of the title compound in the gas phase using the DFT/HF 6-31G(d) level. In addition, E_{LUMO}-E_{HOMO}

energy gap (ΔEg), electronegativity (χ), electron affinity (A), global hardness (η), softness (S), ionization potential (I), chemical potential (Pi), electrophilic index(ω), Nucleophilic index (IP), total energy of the molecule, dipole moments were calculated.

3. RESULTS AND DISCUSSION

3.1 Computational Details

The structural and spectroscopic data of the molecule have been calculated by using DFT/B3LYP and HF 6-31G (d) basis sets at the Gaussian 09W program package on a computing system.

3.2 The R^2 Values of the Compound

B3LYP/DFT 631G(d) (DMSO): [13]C: 0.9936, [1]H: 0.8098.
B3LYP/HF 631G(d) (DMSO): [13]C: 0.9965, [1]H: 0.7917.

Found standard error rate and a, b constants regression values (Table 2) were calculated according to formula exp =a +b. δ calc Eq. Theoretical and experimental carbon and proton chemical shifts ratios between according to R^2 and a, b values, linear a correlation were observed.

Table 1. ^{13}C and ^{1}H-NMR(DMSO) isotropic chemical shifts (δ/ppm)

No	Exp.	DFT/dmso	HF/dmso	Differ/DFT	Differ/HF	No	Exp.	DFT/dmso	HF/dmso	Differ/DFT	Differ/HF
C1	150,28	-5,38	-0,30	145,20	150,28	H15	8,12	-0,67	-0,61	8,06	8,12
C2	152,68	-3,75	2,82	146,11	152,68	H16	7,43	-0,53	-0,38	7,28	7,43
C3	155,38	-3,39	2,93	149,06	155,38	H17	7,12	0,08	-0,19	7,39	7,12
C4	137,24	-9,56	-0,28	127,96	137,24	H18	2,78	-0,54	0,06	2,18	2,78
C5	120,49	-2,36	0,66	117,47	120,49	H19	2,79	-0,55	0,07	2,17	2,79
C6	127,82	-7,93	-0,80	120,69	127,82	H20	2,39	-0,15	0,39	1,85	2,39
C7	147,07	-2,20	6,74	138,13	147,07	H21	2,73	-0,43	0,20	2,10	2,73
C8	154,47	-2,37	7,24	144,86	154,47	H22	2,09	0,21	0,71	1,59	2,09
C9	121,12	6,46	5,77	121,81	121,12	H23	2,86	-0,56	0,13	2,17	2,86
C10	22,96	-11,1	0,01	11,76	22,96	H24	4,49	-0,69	0,74	3,06	4,49
C11	171,45	-2,40	6,97	162,08	171,45	H25	4,10	-0,30	0,25	3,55	4,10
C12	30,50	-9,73	1,12	19,65	30,50	H26	4,22	-0,42	0,10	3,70	4,22
C13	63,20	-6,93	4,95	51,32	63,20	H27	7,12	4,66	5,20	6,58	7,12
C14	10,11	-0,31	0,27	9,53	10,11						

Table 2. The correlation data for chemical shifts of the molecule

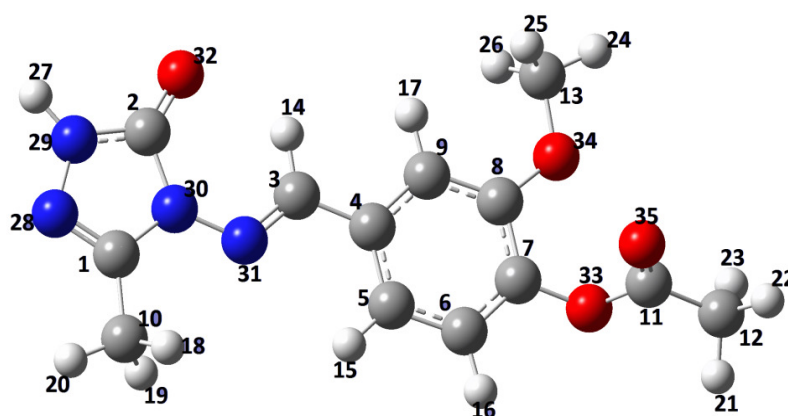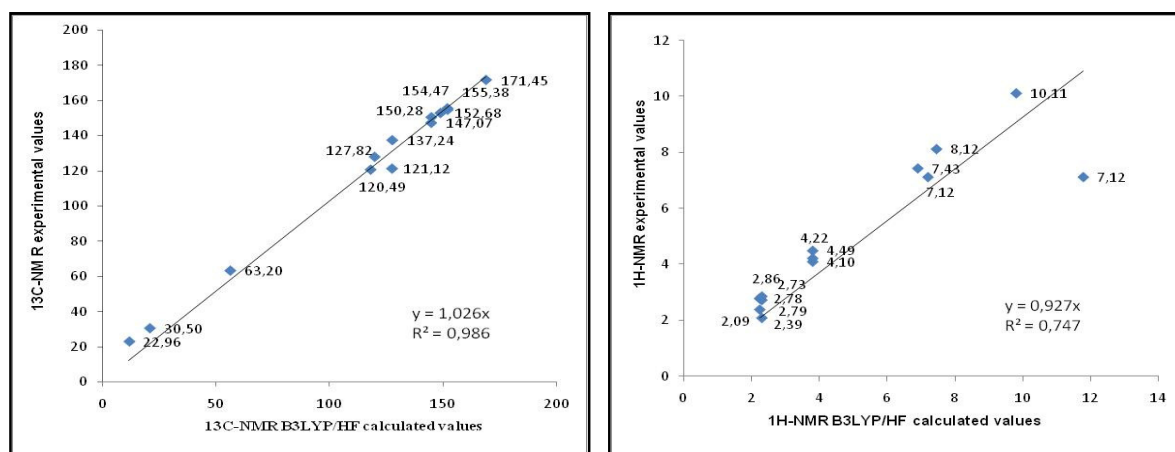|	[13]C				[1]H			
	R	S. error	a	b	R	S. error	a	b
DFT	0.9936	4.1020	1.0497	0.0241	0.8098	1.3907	0.8171	0.1490
HF	0.9965	3.0354	1.0196	0.7097	0.7917	1.4556	0.3320	1.0374

Fig. 1. The Gausview structure of the molecule

Fig. 2. Comparison of experimental and theoretical ^{13}C- and ^{1}H-NMR chemical shifts values of the compound with B3LYP/DFT/HF 631G(d) method

3.3 The Vibration Frequency of the Compound

Theoretically, IR values were calculation veda 4f programme and scala values were obtained. Theoretical calculated IR data are multiplied with appropriate adjustment factors respectively 0.9613, 0.8929 for DFT/631G(d), HF/631G(d) basis sets. The negative frequency in the data was not found. IR spectrums were drawn with obtained values according to HF and DFT method. Theoretically calculated IR values were compared with experimental IR values and found to be compatible with each other.

3.4 Molecular Geometry

The molecular geometric parameters such as bond lengths, bond angles, Mulliken atomic charges calculated by using the HF and DFT/B3LYP methods with 6-31G(d) basis set,

obtained data are a precondition in Tables 4-6. According to this result, the N28-N29, N28-C1, C2-O32, N29-C2 bond lengths in the triazole ring are calculated with DFT/HF 6-31G(d) methods 1.38/1.37, 1.30/1.26, 1.22/1.20, 1.37/1.34 Å (Table 4). In the literature, the N=C, N-N, C=O bond lengths are measured as 1.280, 1.404, 1.212 Å [24,25]. The highest bond angle is between N(29)-C(2)-O(32) atoms, which is 129.92/129.46^{0} (Table 5). The calculated Mulliken atomic charges [26] calculated by using the Hartree Fock (HF) and DFT/B3LYP methods with 6-31G(d) basis sets. The electronegative oxygen (O) and nitrogen (N) atoms have negative atomic charge values. The carbon atoms surrounded by electronegative atoms have positive atomic charge values. The C1 atom surrounded by two electronegative atoms (N28, N29) and C2 atom which is surrounded by three electronegative atoms (N29, N30, O32) have the highest positive charges values. All

hydrogen atoms of the compound (**3**) have positive atomic charge values (Table 6).

Table 3. Significant vibrational frequencies (cm^{-1})

Vibration	Experimental	Theoretical
v (NH)	3183	3850
v (C=O)	1770, 1700	1742
v (C=N)	1596, 1578	1648
v (COO)	1267	1324

3.5 Frontier Molecular Orbital Analysis

Frontier molecular orbitals (FMO) (Figs. 4, 5) determines the electric, electronic transitions, optical properties and kinetic stability [27]. HOMO-LUMO energy of compound was calculated using B3LYP/DFT 6-31G (d) level of theory. The HOMO-LUMO energy gap is 4.31 e.v. for B3LYP/DFTbasis set and 10.79 e.v. for B3LYP/HF 6-31G (d,p) basis set (Fig. 4). Using HOMO-LUMO energy gap electronegativity (χ),

electron affinity (A), global hardness (η), softness (S), chemical potential (μ), ionization potential (I), chemical potential (Pi), electrophilic index(ω), Nucleophilic index (IP) for the compound was calculated. These all properties are calculated as follows [28-30]:

$$\eta = (I - A)/2, \quad \mu = -(I + A)/2,$$
$$\chi = (I + A)/2, \quad Pi = \chi, \quad \omega = \mu^2 / 2\eta$$

In this formula, I and A symbolised ionization potential and electron affinity of the compound, which are virtually obtained from HOMO and LUMO energies. Where $I = -E_{HOMO}$ and $A = -E_{LUMO}$ showed as per Janak theorem [31] and Perdew et al. [32]. The HOMO-LUMO energy gap in the compound is 4.31; 10.79 e.v. All these parameters such as global hardness (η) chemical potential (μ), the global electrophilicity index (ω), electronegativity (χ), ionization potential (I), chemical potential (Pi), electrophilic index(ω), Nucleophilic index (IP) have been calculated for the target compound using 6-31G (d) basis set and are showed in Table 7.
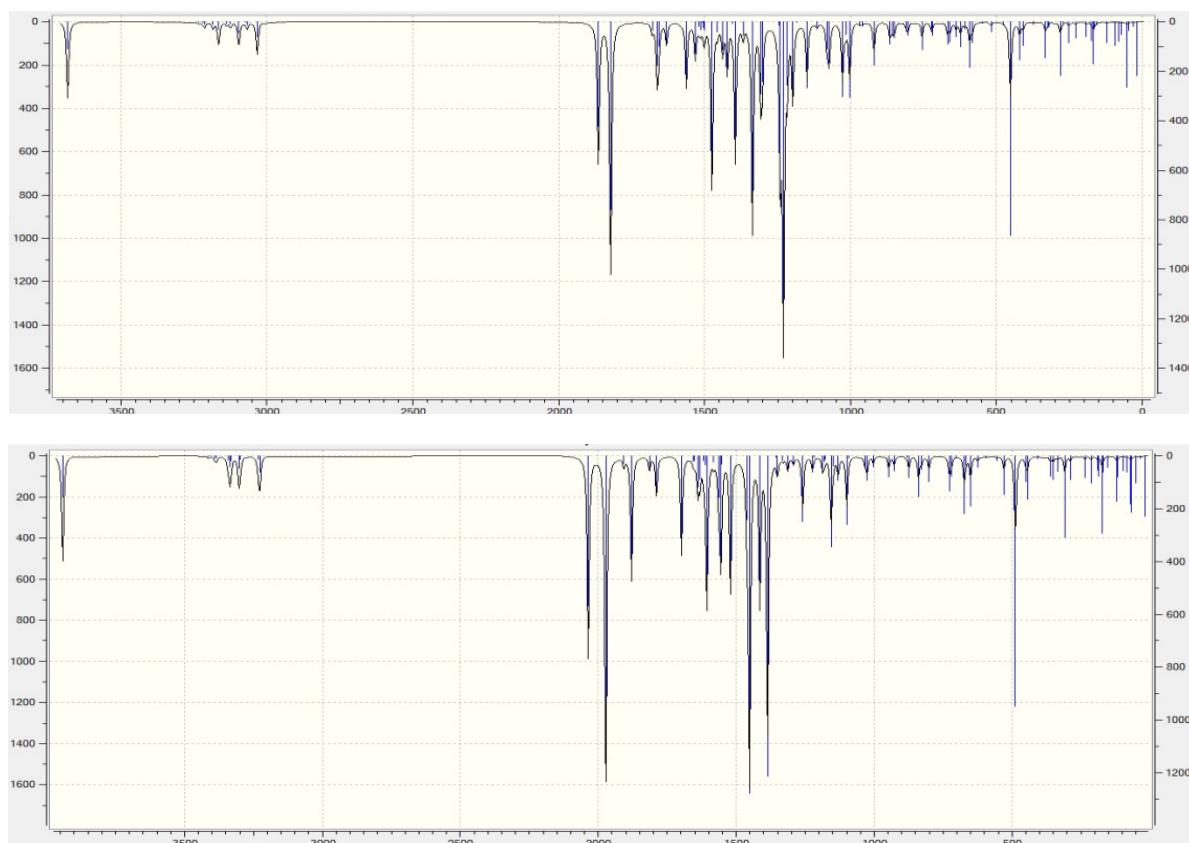

Fig. 3. Theoretical IR spectrums and simulated with DFT/B3LYP/631G(d)(a) and HF/B3LYP/631G(d)(b) levels of the molecule

Table 4. The calculated bond lengths with B3LYP/HF 631G(d) of the molecule

Bond lengths	DFT	HF	Bond lengths	DFT	HF
C(1)-N(28)	1.30	1.26	C(6)-H(16)	1.08	1.07
C(1)-N(30)	1.38	1.37	C(6)-C(7)	1.38	1.38
C(1)-C(10)	1.48	1.48	C(7)-O(33)	1.38	1.37
N(28)-N(29)	1.38	1.37	O(33)-C(11)	1.37	1.34
N(29)-H(27)	1.00	0.99	C(11)-O(35)	1.20	1.18
N(29)-C(2)	1.37	1.34	C(11)-C(12)	1.50	1.50
C(2)-N(30)	1.41	1.38	C(12)-H(21)	1.09	1.08
C(2)-O(32)	1.22	1.20	C(12)-H(22)	1.09	1.08
N(30)-N(31)	1.37	1.36	C(12)-H(23)	1.09	1.08
C(10)-H(18)	1.09	1.08	C(7)-C(8)	1.40	1.38
C(10)-H(19)	1.09	1.08	C(8)-O(34)	1.35	1.35
C(10)-H(20)	1.09	1.08	O(34)-C(13)	1.42	1.41
N(31)-C(3)	1.28	1.25	C(13)-H(24)	1.09	1.08
C(3)-H(14)	1.08	1.07	C(13)-H(25)	1.09	1.08
C(3)-C(4)	1.46	1.47	C(13)-H(26)	1.09	1.08
C(4)-C(5)	1.40	1.39	C(8)-C(9)	1.39	1.38
C(5)-H(15)	1.08	1.07	C(9)-H(17)	1.08	1.07
C(5)-C(6)	1.39	1.38			

Table 5. The calculated bond angles with B3LYP/HF 631G(d) of the molecule

Bond angles	B3LYP	HF	Bond angles	B3LYP	HF
N(28)-C(1)-N(30)	111,45	111.30	C(6)-C(7)-O(33)	119,23	118,65
N(28)-N(29)-H(27)	120,26	120,78	O(33)-C(11)-O(35)	123,74	123,77
H(27)-N(29)-C(2)	125,15	125.41	O(35)-C(11)-C(12)	126,65	125,81
N(29)-C(2)-O(32)	129,92	129,46	C(11)-C(12)-H(21)	110,55	110,00
O(32)-C(2)-N(30)	128,95	128,67	C(11)-C(12)-H(22)	109,44	109,52
N(30)-C(1)-C(10)	123,41	123,26	C(11)-C(12)-H(23)	109,38	109,20
C(1)-C(10)-H(18)	111,04	110,59	H(21)-C(12)-H(22)	110,31	110.26
C(1)-C(10)-H(19)	111,04	110,59	H(21)-C(12)-H(23)	107,43	107,75
C(1)-C(10)-H(20)	108,67	108,60	H(22)-C(12)-H(23)	109,66	110,05
C(1)-N(30)-C(2)	108,38	108,15	C(7)-C(8)-O(34)	116,12	118,41
N(30)-N(31)-C(3)	118,66	119,81	C(8)-O(34)C(13)	118,16	117,35
N(31)-C(3)-H(14)	121,88	122,32	O(34)-C(13)-H(24)	105,76	106,22
H(14)-C(3)-C(4)	117,81	117,32	O(34)-C(13)-H(25)	111,32	110,61
C(3)-C(4)-C(5)	122,63	122,52	O(34)-C(13)-H(26)	111,46	111.30
C(3)-C(4)-C(9)	117,71	117,97	H(24)-C(13)-H(25)	109,43	109,70
C(4)-C(5)-H(15)	119,52	119,86	H(24)-C(13)-H(26)	109,31	110,01
C(4)-C(5)-C(6)	119,68	119,74	H(25)-C(12)-H(26)	109,45	108,87
C(4)-C(8)-C(9)	120,83	121,01	C(7)-C(8)-C(9)	118,52	118,61
C(5)-C(6)-H(16)	121,20	121,07	O(34)-C(8)-C(9)	125,34	122,93
C(5)-C(6)-C(7)	120,39	120,20	C(8)-C(9)-H(17)	120,26	119,09
H(16)-C(6)-C(7)	118,39	118,71			

3.6 Investigation of Thermodynamics Properties of the Compound

Thermodynamics parameters of molecule calculated with B3LYP/DFT 631G (d) and B3LYP/HF 631G (d) basis sets. The thermodynamic data provide helpful information for the further study on the molecule, when these may be used as a reactant to take part in a new reaction. Thermodynamic parameters of the molecule (such as thermal energy, zero-point, vibrational energies (ZPVE), heat capacity, entropy, rotational temperatures and rotational constants) were calculated 298.150 K and 1 atm of pressure. In addition to, the standard thermodynamic functions of heat capacity CV^0, entropy S^0 and enthalpy H^0 were obtained at the B3LYP/DFT/HF 631G(d) level and listed in Table 8. Also, dipole moments, total energy values of the studied compound were calculated by using

B3LYP/DFT/HF 6-31G(d) method in the gas phase. The dipole moments occur when there is a separation of positive and negative charges and ıt is a measure of the polarity of the molecule. The calculated dipole moment is found to be 3.9797 and 5.0066 a.u. for B3LYP/DFT/HF 6-31G(d) basis sets. The direction of the dipole moment is mainly carried out for the z axis (μ_z=1.337 and 1.793 a.u). It can be seen from Table 9. The total energy values of the molecule were calculated -1023.6860 and -1017.6564 for B3LYP/DFT/HF 6-31G(d) basis sets and are given in Table 10.

3.7 Molecular Electrostatic Potantial, Electron Spin Potantial, Total Density and Contour Maps

The molecular electrostatic potential (MEP) is concerned the electronic density and is a very useful definer for designate sites for electrophilic attack and nucleophilic reactions as well as hydrogen-bonding interactions [33-35]. The colour scheme for the MEP surface is as follows: red for electron rich, partially negative charge; blue for electron deficient, partially positive charge; light blue for the slightly electron deficient region; yellow for the slightly electron rich region; green for neutral; respectively [36,37]. In other words, electrostatic potential increases in the order red < orange < yellow < green < blue [38]. The contour map (Electron Density, Electrostatic Potantial), the total density, the Electron Spin Potantial (ESP) have been calculated by same basis sets at 0.004 density values at the same level of calculations of the MEP mapped surface of the molecule and the calculated molecular surfaces of the molecule given in Fig. 5.

Table 6. The calculated mulliken charges data B3LYP/HF 631G(d) of the molecule

	DFT	HF		DFT	HF
C1	0.544	0.607	H19	0.182	0.203
C2	0.822	1.057	H20	0.184	0.212
C3	0.030	0.092	H21	0.183	0.203
C4	0.148	-0.020	H22	0.184	0.208
C5	-0.180	-0.200	H23	0.190	0.211
C6	-0.166	-0.225	H24	0.175	0.192
C7	0.326	0.373	H25	0.164	0.184
C8	0.380	0.410	H26	0.156	0.154
C9	-0.277	-0.274	H27	0.356	0.419
C10	-0.508	-0.523	N28	-0.321	-0.337
C11	0.606	0.772	N29	-0.520	-0.661
C12	-0.528	-0.571	N30	-0.412	-0.619
C13	-0.218	-0.183	N31	-0.313	-0.314
H14	0.207	0.289	O32	-0.542	-0.657
H15	0.152	0.236	O33	-0.525	-0.671
H16	0.145	0.226	O34	-0.442	-0,676
H17	0.148	0.232	O35	-0.514	-0,551
H18	0.183	0.203			

Table 7. The calculated electronic structure parameters of the molecule

		Hatree	ev	kcal/mol	KJ/mol
	LUMO	-0,0571	-1,55373	-35,8304	-149,916
	HOMO	-0,21502	-5,85084	-134,926	-564,535
A	Electron Affinity	0,0571	1,55373	35,8304	149,916
I	Ionization Potential	0,21502	5,85084	134,926	564,535
ΔE	Energy Gap	0,15792	4,29711	99,0953	414,619
χ	Electronegativity	0,13606	3,70229	85,3781	357,226
Pi	Chemical Potential	-0,13606	-3,70229	-85,3781	-357,226
ω	Electrophilic İndex	0,000730867	0,01989	0,45862	1,91889
IP	Nucleophilic İndex	-0,0107433	-0,29233	-6,74145	-28,2065
S	Molecular Softness	12,6646	344,614	7947,1	33251
η	Molecular Hardness	0,07896	2,14856	49,5476	207,309

DFT$_{LUMO}$

E$_{lumo}$= -1.54 eV

△E = 4.31 eV

E$_{homo}$= -5.85 eV

DFT$_{HOMO}$

HFLUMO

E$_{lumo}$= 2.31 eV

△E = 10.79 eV
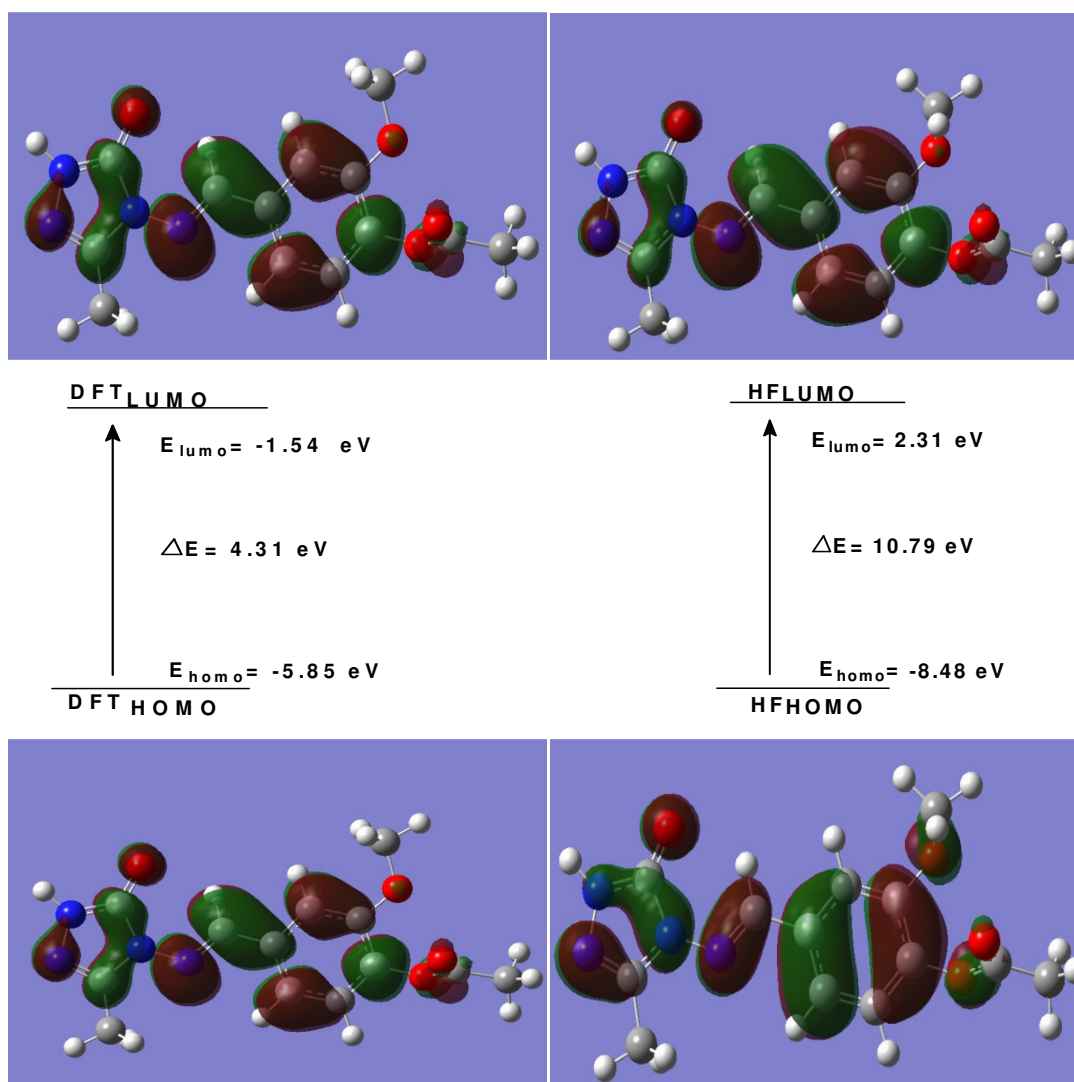
E$_{homo}$= -8.48 eV

HFHOMO

Fig. 4. HOMO-LUMO energy of the molecule

Table 8. The calculated thermodynamics parameters of the molecule

Rotational temperatures (Kelvin)	DFT	HF
A	0.03892	0.04167
B	0.00564	0.00566
C	0.00506	0.00511
Rotational constants (GHZ)		
A	0.81086	0.86834
B	0.11753	0.11789
C	0.10544	0.10656
Thermal energies E(kcal/mol)		
Translational	0.889	0.889
Rotational	0.889	0.889
Vibrational	179.864	192.267
Total	181.641	194.044
Thermal capacity CV(cal/mol-K)		
Translational	2.981	2.981
Rotational	2.981	2.981
Vibrational	67.649	62.892
Total	73.611	68.853

| Rotational temperatures (Kelvin)	DFT	HF
Entropy S(cal/mol-K)		
Translational	42.893	42.893
Rotational	34.724	34.643
Vibrational	74.552	70.634
Total	152.169	148.170
Zero-point correction (Hartree/Particle)	0.269204	0.289975
Thermal correction to Energy	0.289463	0.309229
Thermal correction to Enthalpy	0.290408	0.310173
Thermal correction to Gibbs Free Energy	0.218107	0.239773
Sum of electronic and zero-point Energies	-1023.416818	- 1017.366466
Sum of electronic and thermal Energies	-1023.396558	- 1017.347212
Sum of electronic and thermal Enthalpies	-1023.395614	- 1017.346268
Sum of electronic and thermal Free Energies	-1023.467914	- 1017.416668
Zero-point vibrational energy (Kcal/mol)	168.92780	181.96175
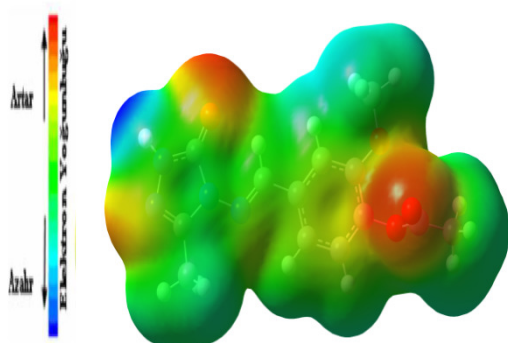
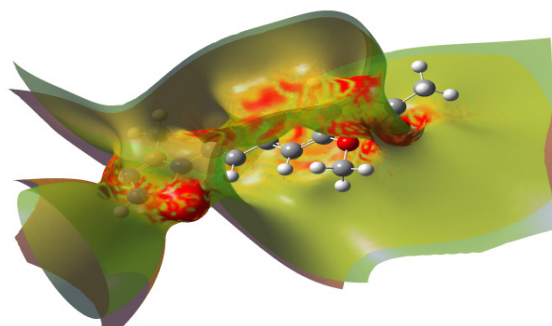**The MEP of the molecule**
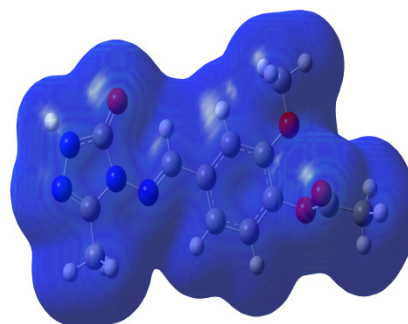
The Total density of the molecule
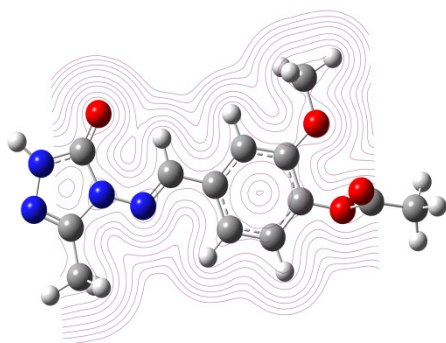
The Electron Density of the molecule
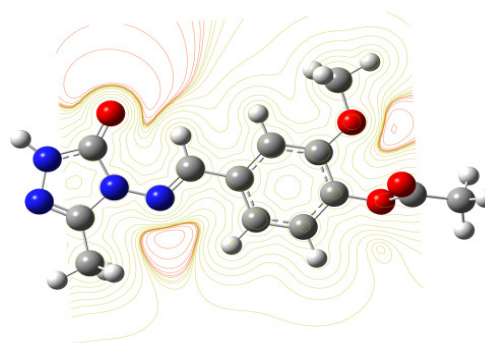
The Electrostatic Potential of the molecule

The ESP of the molecule

Fig. 5. The calculated molecular surfaces of the molecule

Table 9. The calculated dipole moments data of the molecule

	μ_x	μ_y	μ_z	μ_{Toplam}
Dft	-0.0581	-3.7480	1.3370	3.9797
Hf	-0.3876	-4.6583	1.7933	5.0066

Table 10. The calculated total energy data B3LYP/HF of the molecule

Enerji (a.u.)	DFT	HF
	-1023.6860	-1017.6564

4. CONCLUSION

In this work, electronic, geometric and spectroscopic parameters of the molecule are calculated by Density Functional Theory (DFT) and Hartree-Fock (HF) methods with the 631G(d) basis sets of the program package Gaussian G09W. Obtained spectroscopic parameters are compared with experimental data. In addition, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), bond angles, bond lengths, mulliken charges, E_{LUMO}-E_{HOMO} energy gap (ΔEg), electronegativity (χ), electron affinity (A), global hardness (η), softness (σ), ionization potential (I), total energy of the molecule, thermodynamics properties, dipole moments were calculated with B3LYP/DFT631G (d) and HF/631G (d) basis sets. Furthermore, IR vibrational frequencies and IR spectrums were obtained. The IR data was found positive. This result showed that the structure of the compound was stable. The chemical shifts in the calculations ^{1}H-NMR and ^{13}C-NMR and IR vibrational frequencies are found to be compatible with the experimental data. Theoretical and experimental carbon and proton chemical shifts ratios between according to a, b and R^2 values, linear a correlation were observed.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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